Theoretical Study of Temporal Evolution of Ni-Al-Cr Alloys by Kinetic Monte Carlo Simulations

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- **Precipitation and ordering in Ni-Al-Cr alloys are studied by kinetic Monte Carlo (KMC) simulations.**

- **The mechanism of KMC is the thermally activated migration of atoms by a vacancy jumping to first nearest-neighbor sites in a rigid FCC lattice employing a residence time algorithm.**

- **In the early stages (<1 hour), both phase separation and ordering develop and both Ni_3Cr and Ni_3Al $L1_2$ co-exist. At later stages, the Al-rich ordered phase develops, resulting in the volume fraction of the $L1_2$ γ' phase increasing with aging time.**

- **The results of KMC simulations are in excellent agreement with our three-dimensional atom-probe experimental results.**

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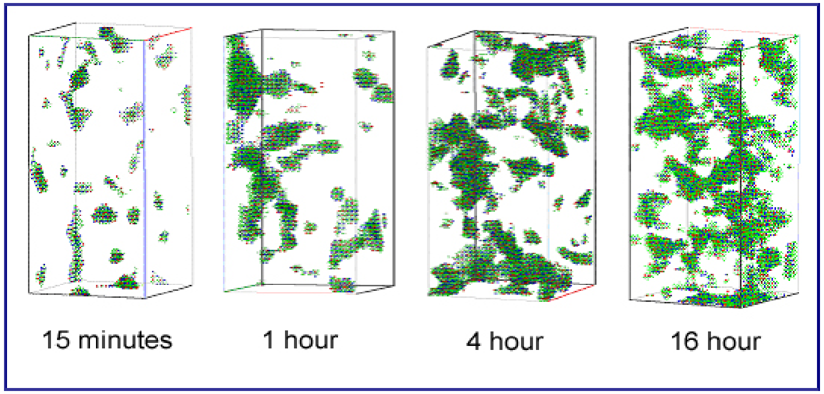

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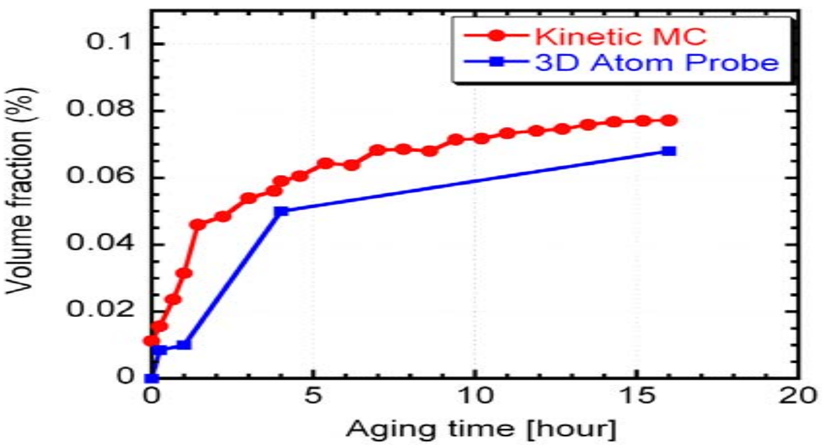

***1*. The simulated evolution of γ' phase in Ni-5.24 at.% Al-14.24 at.% Cr alloy vs. aging time by KMC simulations at 600°C.**

***2*. The volume fraction of γ' phase as function of aging time compared with experimental results.**

Nanoscale studies of the chemistry of a René N6 superalloy

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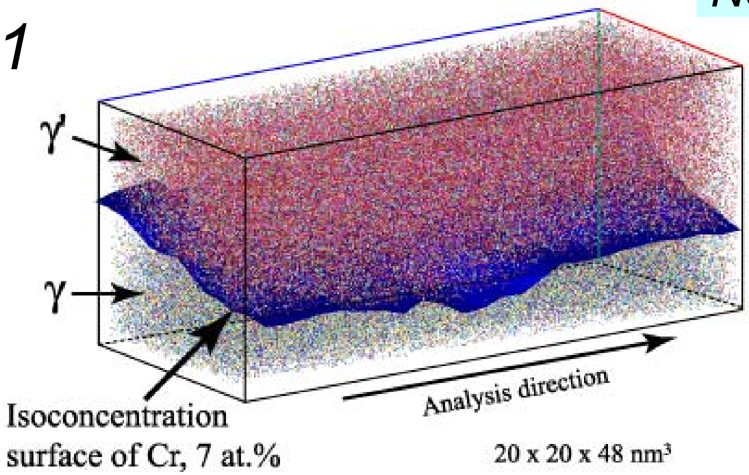

1 Three-dimensional atom-by-atom reconstruction of René N6 superalloy, showing γ/γ' interface.

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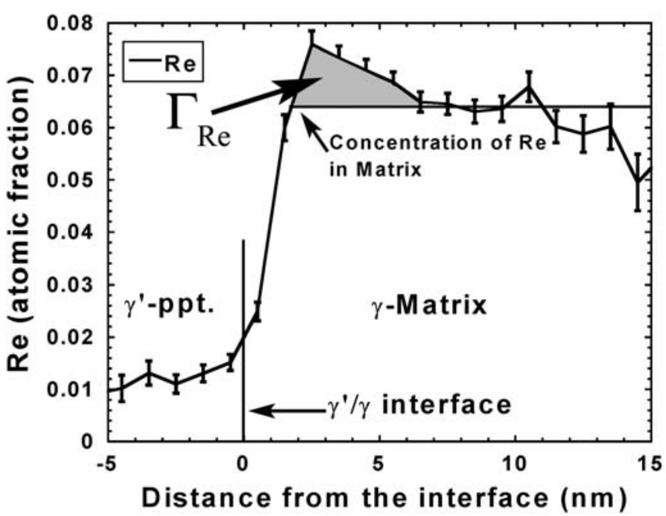

- **Third generation Ni-based superalloy developed by General Electric Aircraft Engines.**
- **Complex commercial alloy that contains nine elements – Ni, Cr, Al, Co, Ta, Mo, Re, W, Hf**
- **Material extensively used for turbine engine blades**
- **High corrosion and creep resistance at elevated temperatures**
- **Subnanometer scale chemical study is performed using three-dimensional atom probe (3DAP).**
- **Segregation of Re observed at γ-matrix (FCC)/γ'-precipitates ($L1_2$) interface - 2.46 ± 0.68 atoms nm^{-3}.**
- **Addition of Re in Ni-based superalloy increases creep resistance at high temperature.**

2 **Determination of the Gibbsian interfacial excess using proxigram generated by *ADAM,* software developed at NU for analyzing data collected by 3DAP.**

The proximity histogram (or proxigram for short) method is a data analysis technique we have developed to generate isoconcentration profiles with respect to internal interfaces in a geometrically independent way. This analysis technique integrates the chemical and three-dimensional positional information and then generates simultaneously an atomic fraction versus distance to interface histogram for all the interfaces in a specimen delineated by this isoconcentration surface. In addition, it does not require choosing any arbitrary axis or geometric subvolume. Therefore, the proxigram can be used to generate in parallel, for all the interfaces in a specified volume of material, a concentration profile for large data sets, and thereby readily detects Gibbsian interfacial excess values for all the precipitate/matrix interfaces in an analyzed volume.

A third-generation Ni-based superalloy, René N6, which has been developed by General Electric Corporation, was investigated by three-dimensional atom probe (3DAP) microscopy at Northwestern University. Approximately 1.4 million ions were collected from one sample and data analyses were performed using *ADAM* 1.5 (Fig. 1), a custom Macintosh application we developed to analyze data generated by our 3DAP microscope. Segregation of Re at the γ/γ' interface was observed and the Gibbsian interfacial excess was determined (2.46 ± 0.68 atoms nm^{-3}) using the proxigram method, Fig. 2. Due to the calculation technique the proxigram method employs, it is applicable to both planar and non-planar heterophase interfaces. In addition, this makes the sensitivity of the measured excess value on the threshold value to be small as shown for this system.

Segregation at Molybdenum Nitride/ α-Fe Interfaces

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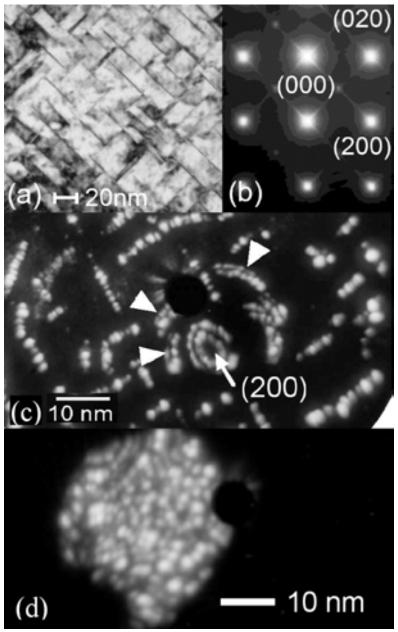
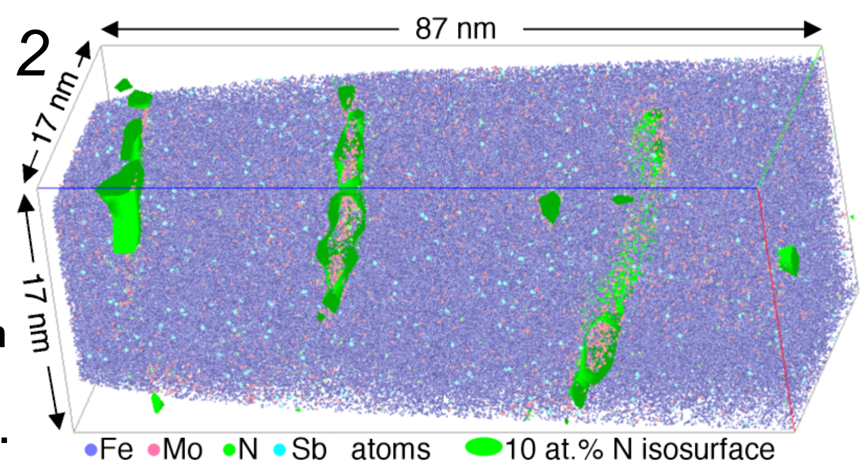


- **Finely dispersed precipitates, such as Mo_3N_2, produced by internal nitridation of an Fe alloy, efficiently harden the alloy.**
- **We study segregation of solute atoms at coherent and semicoherent molybdenum/α–Fe heterophase interfaces.**
- **Combination of transmission electron (TEM), field-ion (FIM) and three-dimensional atom-probe (3DAP) microscopies allows for atomic-scale characterization of atomic structure and chemistry.**
- **Segregation of tin and antimony is found to be much larger at semicoherent interfaces of coarser molybdenum nitride precipitates as compared to coherent interfaces of smaller ones.**

1 **Coherent, thin molybdenum nitride platelets as seen by TEM (a),(b) and FIM (c); and FIM of a semicoherent, spherical precipitate (d).**

2 **The platelets are delineated by the 10 at.% nitrogen isoconcentration surface based on an atom-by-atom 3DAPM reconstruction, utilizing *ADAM*, visualization software developed at NU.**

2



Molybdenum Nitride Platelets in α-Fe

Temporal Evolution of the Microstructure in Nickel -based Superalloys

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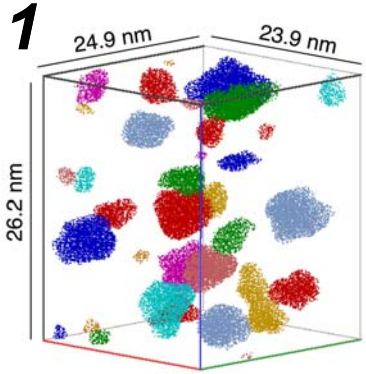


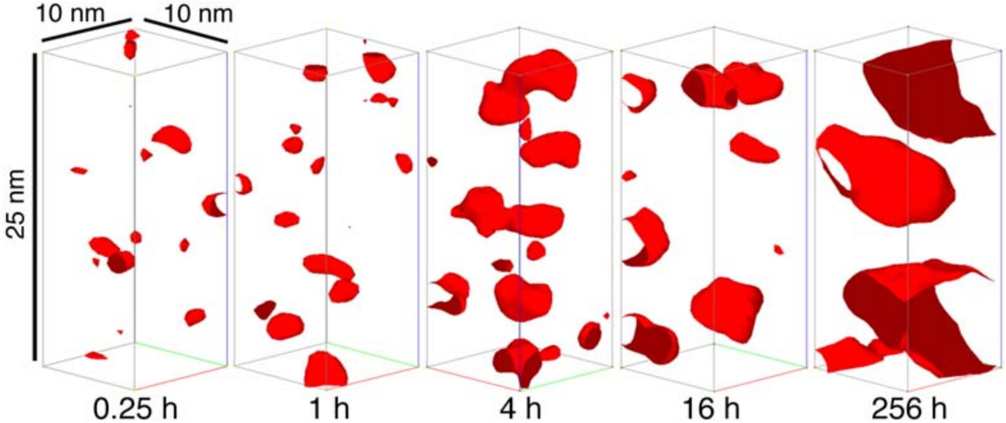
Nanoscale Ni_3Al precipitates

- **Technologically relevant, superalloys combine high strength and corrosion resistance. Their primary use is for turbine blades in jet engines.**
- **Ni- based superalloys derive their excellent mechanical properties from the presence of Ni_3Al precipitates within the face-centered cubic matrix.**
- **With subnanoscale resolution, we investigate the temporal evolution of the microstructure (Ni_3Al precipitates) in model Ni-based superalloys.**
- **The confluence of experiment and simulation provides a full chemical and structural understanding from the earliest to late stages of development.**
- **Experimental images presented are atom-by-atom reconstructions of the lattice with spatial and chemical information for each atom.**

1 **Utilizing *ADAM*, visualization software developed at NU, individual Ni_3Al precipitates are detected and analyzed.**

2 **The 9 at. % Al isoconcentration surface in red describes the evolving microstructure with time. Individual atoms are omitted for clarity.**

2



Growth of Ni_3Al precipitates evolving with time

Atomic Scale Studies of Heterophase Interfaces

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- **Current post-graduate research participants: 2 graduate students performing experiments (Chantal Sudbrack, Kevin Yoon), and 1 research associate (Dieter Isheim). 1 research associate performing simulation /theory (Zugang Mao).**

- **18 past and current undergraduate REU, work-study and senior project students participating in experiments (Jenny Andrew, Maryjoy Carnate, Yat-Kiu Fung, Mark Greene, Cynthia Herrara, Anna Jozwik, Mark Murphey, Michael Potter, Adam Pyzyna, Ellen Siem, Stephen Sharon, Ie Uttayarat, Mark White,Tiffany Ziebell), and participating in development of software code, *ADAM*, for analysis of three-dimensional atom-probe (3DAP) data (John Blatz du Rivage, Joel Flaxman, Joshua Paul, Justin Vandenbroucke).**

Graduate student, Chantal Sudbrack (right), instructs REU student, Maryjoy Carnate (left), in electropolishing specimens for the 3D atom-probe.

OUTREACH (by Dr. Olof C. Hellman, research associate)

- **Development of a program, Cahn Man, to simulate Cahn-Hilliard theory of spinodal decomposition. Used for teaching sophomores and juniors phase transformations at NU.**

- **Development of a program, kSan, to teach simple crystallography and atomic structure of grain boundaries. Used by sophomores, juniors, and graduate students at NU.**

- **Involved Evanston Township High School students in the development of a software code, *ADAM*, for analyzing three-dimensional atom-probe (3DAP) data.**